

# SAFETY DATA SHEETS

According to the UN GHS revision 9

Version: 1.0  
Creation Date: July 15, 2019  
Revision Date: July 15, 2019

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## SECTION 1: Identification

### 1.1 GHS Product identifier

**Product name** Theophylline

### 1.2 Other means of identification

**Product number** -  
**Other names** [13C]-Theophyllin; Unifyl; 3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione

### 1.3 Recommended use of the chemical and restrictions on use

**Identified uses** Industrial and scientific research use.  
**Uses advised against** no data available

### 1.4 Supplier's details

**Company** Shanghai Yien Chemical Technology Co., Ltd  
**Address** Building 6, 28 Yingong Road, Fengxian District, Shanghai  
Chemical Industry Zone, Shanghai, 201400, China  
**Telephone** +86-400-133-2688

### 1.5 Emergency phone number

**Emergency phone number** +86-400-133-2688  
**Service hours** Monday to Friday, 9am-5pm (Standard time zone: UTC/GMT +8 hours).

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## SECTION 2: Hazard identification

### 2.1 Classification of the substance or mixture

Acute toxicity - Category 3, Oral

### 2.2 GHS label elements, including precautionary statements

**Pictogram(s)**



**Signal word** Danger  
**Hazard statement(s)** H301 Toxic if swallowed  
**Precautionary statement(s)**  
**Prevention** P264 Wash ... thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
**Response** P301+P316 IF SWALLOWED: Get emergency medical help

**Storage** immediately.  
**Disposal** P321 Specific treatment (see ... on this label).  
P330 Rinse mouth.  
P405 Store locked up.  
P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

### 2.3 Other hazards which do not result in classification

no data available

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Chemical name	Common names and synonyms	CAS number	EC number	Concentration
Theophylline	Theophylline	58-55-9	200-385-7	100%

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## SECTION 4: First-aid measures

### 4.1 Description of necessary first-aid measures

#### If inhaled

Fresh air, rest.

#### Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower.

#### Following eye contact

Rinse with plenty of water for several minutes (remove contact lenses if easily possible).

#### Following ingestion

Rinse mouth. Give a slurry of activated charcoal in water to drink. Refer for medical attention .

### 4.2 Most important symptoms/effects, acute and delayed

no data available

### 4.3 Indication of immediate medical attention and special treatment needed, if necessary

no data available

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## SECTION 5: Fire-fighting measures

### 5.1 Suitable extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

### 5.2 Specific hazards arising from the chemical

Not combustible. Gives off irritating or toxic fumes (or gases) in a fire.

### 5.3 Special protective actions for fire-fighters

In case of fire in the surroundings, use appropriate extinguishing media.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Personal protection: particulate filter respirator adapted to the airborne concentration of the substance. Sweep spilled substance into sealable containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

## 6.2 Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

## 6.3 Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

### 7.2 Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs.

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Occupational Exposure limit values

<b>Component</b>	Theophylline			
<b>CAS No.</b>	58-55-9			
	<b>Limit value - Eight hours</b>		<b>Limit value - Short term</b>	
	<b>ppm</b>	<b>mg/m<sup>3</sup></b>	<b>ppm</b>	<b>mg/m<sup>3</sup></b>
<b>Latvia</b>		0,5		
	<b>Remarks</b>			
<b>Latvia</b>	+ 1,2 Ethylenediamine 107-15-3 Elixophyllin			

#### Biological limit values

no data available

### 8.2 Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### 8.3 Individual protection measures, such as personal protective equipment (PPE)

#### Eye/face protection

Wear safety spectacles.

#### Skin protection

Protective gloves.

#### Respiratory protection

Avoid inhalation of dust and mist.

#### Thermal hazards

no data available

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## SECTION 9: Physical and chemical properties and safety characteristics

<b>Physical state</b>	Solid. Powder.
<b>Colour</b>	White.
<b>Odour</b>	no data available
<b>Melting point/freezing point</b>	270 - 274 °C.
<b>Boiling point or initial boiling point and boiling range</b>	384°C(lit.)
<b>Flammability</b>	no data available
<b>Lower and upper explosion limit/flammability limit</b>	no data available
<b>Flash point</b>	88°C(lit.)
<b>Auto-ignition temperature</b>	610 °C. Atm. press.:1 013 hPa.
<b>Decomposition temperature</b>	no data available
<b>pH</b>	no data available
<b>Kinematic viscosity</b>	no data available
<b>Solubility</b>	In water: 5.5 g/L. Temperature:19.9 °C.
<b>Partition coefficient n-octanol/water</b>	log Pow = -0.008. Temperature:23 °C.
<b>Vapour pressure</b>	0.001 mBar. Temperature:20 °C.
<b>Density and/or relative density</b>	1.36 g/cm <sup>3</sup> . Temperature:25 °C.
<b>Relative vapour density</b>	no data available
<b>Particle characteristics</b>	no data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

no data available

### 10.3 Possibility of hazardous reactions

Decomposes on heating. This produces toxic fumes including nitrogen oxides.

### 10.4 Conditions to avoid

no data available

### 10.5 Incompatible materials

no data available

### 10.6 Hazardous decomposition products

no data available

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## SECTION 11: Toxicological information

### Acute toxicity

- Oral: LD50 - rat (female) - 272 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - > 6.7 mg/L air.
- Dermal: LD50 - rat (male/female) - > 2 000 mg/kg bw.

### Skin corrosion/irritation

no data available

### Serious eye damage/irritation

no data available

**Respiratory or skin sensitization**

no data available

**Germ cell mutagenicity**

no data available

**Carcinogenicity**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

The substance may cause effects on the heart and central nervous system. This may result in cardiac dysrhythmia and convulsions. The effects may be delayed.

**STOT-repeated exposure**

no data available

**Aspiration hazard**

A nuisance-causing concentration of airborne particles can be reached quickly when dispersed.

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**SECTION 12: Ecological information**

**12.1 Toxicity**

- Toxicity to fish: LC50 - *Leuciscus idus* - 100 mg/L - 96 h.
- Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna* - 178 mg/L - 48 h.
- Toxicity to algae: EC50 - *Desmodesmus subspicatus* (previous name: *Scenedesmus subspicatus*) - > 100 mg/L - 72 h.
- Toxicity to microorganisms: EC80 - activated sludge - > 1 000 mg/L - 180 min.

**12.2 Persistence and degradability**

no data available

**12.3 Bioaccumulative potential**

no data available

**12.4 Mobility in soil**

no data available

**12.5 Other adverse effects**

no data available

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**SECTION 13: Disposal considerations**

**13.1 Disposal methods**

**Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

**Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and

then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

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## SECTION 14: Transport information

### 14.1 UN Number

ADR/RID: UN1544 (For reference only, please check.)      IMDG: UN1544 (For reference only, please check.)      IATA: UN1544 (For reference only, please check.)

### 14.2 UN Proper Shipping Name

ADR/RID: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)      IMDG: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)      IATA: ALKALOIDS, SOLID, N.O.S. or ALKALOID SALTS, SOLID, N.O.S. (For reference only, please check.)

### 14.3 Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)      IMDG: 6.1 (For reference only, please check.)      IATA: 6.1 (For reference only, please check.)

### 14.4 Packing group, if applicable

ADR/RID: I (For reference only, please check.)      IMDG: I (For reference only, please check.)      IATA: I (For reference only, please check.)

### 14.5 Environmental hazards

ADR/RID: No      IMDG: No      IATA: No

### 14.6 Special precautions for user

no data available

### 14.7 Transport in bulk according to IMO instruments

no data available

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## SECTION 15: Regulatory information

### 15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
Theophylline	Theophylline	58-55-9	200-385-7
European Inventory of Existing Commercial Chemical Substances (EINECS)			Listed.
EC Inventory			Listed.
United States Toxic Substances Control Act (TSCA) Inventory			Listed.
China Catalog of Hazardous chemicals 2015			Not Listed.
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Listed.
Chinese Chemical Inventory of Existing Chemical Substances (China IECSC)			Listed.
Korea Existing Chemicals List (KECL)			Listed.

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## SECTION 16: Other information

### Information on revision

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## Abbreviations and acronyms

- CAS: Chemical Abstracts Service
- ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road
- RID: Regulation concerning the International Carriage of Dangerous Goods by Rail
- IMDG: International Maritime Dangerous Goods
- IATA: International Air Transportation Association
- TWA: Time Weighted Average
- STEL: Short term exposure limit
- LC50: Lethal Concentration 50%
- LD50: Lethal Dose 50%
- EC50: Effective Concentration 50%

## References

- IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: [http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

**Any questions regarding this SDS, Please send your inquiry to [sds@xixisis.com](mailto:sds@xixisis.com)**

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*Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any damage resulting from handling or from contact with the above product.*